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The internal structure of igniting turbulent sprays as revealed by complex chemistry DNS

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ABSTRACT

A parametric study of spark ignition in a uniform monodisperse turbulent spray is performed with complex chemistry three-dimensional Direct Numerical Simulations in order to improve the understanding of the structure of the ignition kernel. The heat produced by the kernel increases with the amount of fuel evaporated inside the spark volume. Moreover, the heat sink by evaporation is initially higher than the heat release and can have a negative effect on ignition. With the sprays investigated, heat release occurs over a large range of mixture fractions, being high within the nominal flammability limits and finite but low below the lean flammability limit. The burning of very lean regions is attributed to the diffusion of heat and species from regions of high heat release, and from the spark, to lean regions. Two modes of spray ignition are reported. With a relatively dilute spray, nominally flammable material exists only near the droplets. Reaction zones are created locally near the droplets and have a non-premixed character. They spread from droplet to droplet through a very lean interdroplet spacing. With a dense spray, the hot spark region is rich due to substantial evaporation but the cold region remains lean. In between, a large surface of flammable material is generated by evaporation. Ignition occurs there and a large reaction zone propagates from the rich burned region to the cold lean region. This flame is wrinkled due to the stratified mixture fraction field and evaporative cooling. In the dilute spray, the reaction front curvature pdf contains high values associated with single droplet combustion, while in the dense spray, the curvature is lower and closer to the curvature associated with gaseous fuel ignition kernels.

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1. Introduction

Valuable physical background can be obtained by studying spark ignition in a uniformly-distributed monodisperse spray. The knowledge extracted can help understanding ignition in realistic flows involving sprays. The factors that control ignition success in laminar and turbulent uniform monodispersed droplets have been investigated in the past [1–3]. The general model developed by Ballal and Lefebvre [4] to determine the Minimum Ignition Energy (MIE) in overall lean sprays matched their experimental data. In the model, the MIE was reduced with higher evaporation rate and lower turbulence intensity, consistent with previous investigations [2,5–9]. This model was based on the assumption that droplets burn individually and that heat release is determined by the theory of single droplet combustion [4]. However, this assumption is questionable since no classification of the structure of a spark kernel as a function of droplet parameters has been given. Limited experimental data have suggested that a kernel can still be generated if the spray is very rich [10] and that the kernel grows faster if the gaseous equivalence ratio in the spark is close to stoichiometry [6–8]. However, accurate and simultaneous measurements of quantities of interest (local equivalence ratio, fraction of fuel vapour, species concentration) that help understanding the kernel structure are difficult. Direct Numerical Simulations (DNS) have the potential to improve the current fundamental knowledge of spark ignition in sprays and are the scope of this work. Moreover, the Group Combustion theory and the problem of the flame propagation in a uniform spray can help the interpretation of the results. These are introduced next.

The Group Combustion theory helps determining different modes of combustion for a spherical cloud of droplets surrounded by hot oxidiser [11] based on a Group Combustion number G

$$G = 3\left(1 + 0.276\mathrm{Re}_d^{1/2}\mathrm{Sc}^{1/3}\right)\mathrm{Le}N^{2/3}(a_d/s_d) \quad (1)$$

where Re_d, Sc and Le are respectively the droplet Reynolds number, the Schmidt number and the Lewis number of the fuel vapour. G increases with the total number of droplets N in the cloud and the initial droplet diameter a_d while it decreases with s_d, the mean spacing between droplets. The different regimes range from droplets burning individually for $G \ll 1$, to external sheath combustion for $G \gg 1$ where a flame surrounds the whole droplet cloud [11]. This

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provides useful insight for real applications. For example, it was used to interpret the autoignition of a spherical cloud of droplets in a convective environment [12]. In addition, Aggarwal [2] discussed the different ignition modes following spray auto-ignition and suggested that in turbulent sprays, various Group Combustion regimes could occur locally in the cloud of droplets. Nevertheless, Group Combustion theory does not fully describe the physics of an expanding spray flame. A spherical kernel may have some attributes of Group Combustion, but it also has features of a propagating flame. In premixed gases, the early kernel has been likened to a spherical laminar flame [13]. By analogy, the laminar flame propagation in a uniform spray should contain useful information to understand the structure of a spark kernel.

The flame propagation in a uniform monodisperse spray has undergone extensive investigations where the flame structure was analysed and the flame speed was reported [14–21]. It was observed that inhomogeneities of the mixture fraction at the flame front have a strong effect on the flame propagation. For example, inhomogeneities can result in local diffusion flames around droplets or group of droplets [14,16,21–24]. This can be of favourable consequence in overall lean sprays since heat release can occur at locally stoichiometric mixture fractions. Moreover, it has been observed that the flame front was wrinkled by the presence of the droplets [25,8]. It was suggested that the wrinkling increases the flame surface area and in turn enhances the propagation [25]. Furthermore, it has been suggested by numerous studies that the flame speed could be correlated with the mean gas phase equivalence ratio in the flame reaction zone [19,23,25–27]. Recently, it has also been found that a spray flame has features that can only be captured by detailed chemistry, such as post-flame pyrolysis, and that this could influence to some extent the flame speed [27].

Recent studies have focused on the flame spread in arrays of equally-spaced droplets and have provided additional information on the flame propagation in sprays [28,29]. Under conditions where the fuel existed only in a thin layer near the droplet and the interdroplet spacing contained little or no fuel, these studies reported diffusion flames surrounding droplets. Depending on the interdroplet spacing, different modes of spreading of those diffusion flames were observed and described in Ref. [28]. In their mode 1, the interdroplet spacing is relatively small. The diffusion flame created around one droplet rapidly surrounds the next one and accelerates its evaporation. The higher evaporation rate of this droplet pushes the diffusion flame forward and the flame surrounds the next droplet. In their mode 2, the interdroplet spacing is larger, the diffusion flame created around one droplet reaches the fuel layer evaporated around the next droplet. The fuel layer then ignites and a diffusion flame forms around this droplet. In their mode 3, the interdroplet spacing is even larger. The diffusion flame created around a droplet can only raise the temperature of the next droplet by heat conduction until ignition occurs.

The current knowledge of the structure of an ignition kernel in a spray can be improved by performing DNS simulations with complex chemistry and fully resolved liquid phase. However, resolving liquid phase demands very fine grids, much smaller than the Kolmogorov length scale. This approach has been little adopted since it restricts the size of the domain and the number of droplets [30,31]. It is common practice to use grid size of the order of the Kolmogorov length scale whilst using a point source approximation to model the exchange of mass, momentum and energy between the gas and the droplets [32,33]. This is the approach adopted in this work. However, even with this simplification, complex chemistry 3D DNS of spray ignition and flame propagation has been very limited.

Spark ignition has been studied previously with 1-step chemistry 3D DNS with droplets much smaller than the reaction zone [9,34]. In those studies, it was shown that rapid evaporation of the fuel was necessary for the success of ignition and that the flame propagated in a large range of equivalence ratio due to the mixture stratification. Based on 1-step chemistry 2D DNS, Reveillon and Vervisch [33] have described the propagation of a flame along a jet of dilute fine spray and classified different regimes in a Group Combustion diagram. However, since droplets evaporated very fast compared to the flame front, individually burning droplets were not observed. Furthermore, spark ignition involves high temperatures and a greatly curved kernel. Hence, the role of detailed transport and chemistry is expected to be important. 2D numerical simulations with premixed hydrogen showed that the evolution of the early kernel involved a complicated pattern of secondary species and radicals [35] and that the kernel growth was very sensitive to the thermo-chemical composition [36]. In non-premixed gaseous systems, 2D simulations with methane [37] and with hydrogen [38] also showed that the kernel structure was influenced by differential diffusion and complex chemistry. Moreover, 2D DNS of auto-ignition with *n*-heptane spray and complex chemistry were performed by Wang and Rutland where evaporation cooling was shown to delay the onset of reactions [39,40]. To the authors' knowledge, complex chemistry 3D DNS of spark ignition in sprays was only reported in our previous work [41]. In that paper, the kernel in a uniform volatile spray with an overall equivalence ratio $\phi_0 = 1$ and with a droplet diameter of the order of the stoichiometric laminar reaction zone thickness was presented. The generation and the propagation of local droplet flames were identified and the evolution of species in mixture fraction space showed both non-premixed and partially premixed character [41].

In this paper, the investigation of Ref. [41] is extended and a parametric study on the overall equivalence ratio ϕ_0 and the droplet diameter is presented. Results and figures of Ref. [41] are sometimes referred to for facilitating comparison. In the present paper, different modes of ignition are identified and discussed in the light of Group Combustion Theory and flame propagation in a uniform spray. In the next section, the numerical methods are introduced. Then the results and their discussion are presented. The paper closes with a summary of the main conclusions.

2. Numerical formulation

2.1. Liquid phase

A Lagrangian point-source formulation has been adopted for the liquid phase. Temperature is assumed uniform inside the droplets and droplet–droplet interactions are neglected. A thin film (subscript *f*) assumption is used to calculate the droplet evaporation and heat exchange with the surroundings [42]. This evaporation model [42] is widely used and is recommended since it combines accuracy and efficiency [43].

For each droplet *d*, equations for its position $\mathbf{x}_d$, velocity $\mathbf{v}_d$, diameter a_d and temperature T_d are

$$\frac{d\mathbf{x}_d}{dt} = \mathbf{v}_d \tag{2}$$

$$\frac{d\mathbf{v}_d}{dt} = \frac{\mathbf{U}(\mathbf{x}_d, t) - \mathbf{v}_d}{\tau_d^v} \tag{3}$$

$$\frac{da_d^2}{dt} = -\frac{a_d^2}{\tau_d^p} \tag{4}$$

$$\frac{dT_d}{dt} = \frac{1}{\tau_d^T}\left[T(\mathbf{x}_d, t) - T_d - B_{T,d}\frac{L_v}{W_F C_{P_f}}\left(\frac{T_{crit} - T_d}{T_{crit} - T_{ref}}\right)^{0.38}\right] \tag{5}$$

$\mathbf{U}$ and T are the local gas velocity and temperature. T_{ref} is the boiling temperature at the reference pressure P_{ref}, T_{crit} the critical temperature, L_v the molar latent heat of evaporation and W_F the molecular

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